

# Effective Heisenberg Model and Exchange Interaction for Strongly Correlated Systems

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We consider the extended Hubbard model and introduce a corresponding Heisenberg-like problem written in terms of spin operators. The derived formalism is reminiscent of Anderson's idea of the effective exchange interaction and takes into account nonlocal correlation effects. The results for the exchange interaction and spin susceptibility in the magnetic phase are expressed in terms of single-particle quantities. This fact not only can be used for realistic calculations of multiband systems but also allows us to reconsider a general description of many-body effects in the most interesting physical regimes, where the physical properties of the system are dominated by collective (bosonic) fluctuations. In the strongly spin-polarized limit, when the local magnetic moment is well defined, the exchange interaction reduces to a standard expression of the density functional theory that has been successfully used in practical calculations of magnetic properties of real materials.

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The theory of magnetism is one of the most attractive and discussed areas of physics. Additional interest in this topic is heated up by the theoretical prediction [1] and experimental observation [2–4] of topologically stable Skyrmionic spin textures that are intensively studied now in the context of spintronics and magnetic data storage [5–7]. Also, a correct accounting of spin excitations is important for realization of the Kitaev spin model [8,9] and its practical application in Majorana quantum computers [10–15]. A quantitative description of the mentioned effects requires knowledge of the exchange interaction between two spins. However, this problem is challenging when applied to many magnetic materials that are, by definition, strongly correlated quantum systems.

Originally, the development of the theory of exchange interactions in solids and molecules was based on the Heitler-London theory of the hydrogen molecule [16]. It was demonstrated, however, in the early 1960s by Freeman and Watson [17] that this theory, being applied to ferromagnetic transition metals, gives a completely wrong order of magnitude and even an incorrect sign of the exchange parameters. For magnetic insulators, a semiempirical theory of exchange interactions was developed in the 1950s, known as the Goodenough-Kanamori-Anderson rules [18–21]; however, it was not quantitative. An analysis of “superexchange” in particular compounds always assumed some model considerations, that is, the importance and nonimportance of specific intermediate states. When the density functional theory (DFT) became the base of microscopic quantum theory of molecules and crystals [22–24], the most straightforward way to estimate the exchange interactions was simply the calculation of the

total energy difference between ferromagnetic and antiferromagnetic phases. This assumes the applicability of the Heisenberg model, which is frequently not the case, especially for itinerant electron systems [24–27].

A general, model-independent and parameter-free method to calculate exchange interactions within DFT was suggested in Refs. [28–30] based on the “magnetic local force theorem.” It is based on the consideration of second-order variations of the total energy with respect to small rotations of magnetic moments starting from equilibrium ground states. Later, this approach was generalized to strongly correlated systems [31,32] [within the framework of dynamical mean-field theory (DMFT) [33,34]], magnetic systems out of equilibrium [35], and relativistic magnetic interactions, such as the Dzyaloshinskii-Moriya interaction [36–38]. This theory was successfully used for many calculations of real systems, such as magnetic semiconductors [39], molecular magnets [40,41], ferromagnetic transition metals [42,43], and half-metallic ferromagnets [44].

Despite the success of this approach, its conceptual status remains unclear. Indeed, a mapping from DFT or from a Hubbard model to the Heisenberg model is, in general, impossible; exchange interactions obtained from the magnetic force theorem are classical and dependent on the magnetic configuration (see, e.g., Ref. [45]). Their relation to observables is not very clear; strictly speaking, only the spin-wave stiffness constant in ferromagnets is a well-defined quantity since we can be sure that in the limit of slow times and large spatial scales the phenomenological Landau-Lifshitz equations are correct. This was emphasized already in a previous paper [28]. Observables are

directly related to the dynamic magnetic susceptibility, but to establish relations between the magnetic local force approach and the standard language of response functions is not an easy problem to solve. It was solved only within the local spin-density approximation in DFT [46] and within the time-dependent mean-field approach in the Hubbard model [47]. However, most of the interesting magnetic materials are strongly correlated systems, and these approximations seem to be insufficient (or, at least, not completely justified) to describe spin dynamics.

In this Letter we show that the extended Hubbard Hamiltonian can be mapped onto an effective Heisenberg model. Inspired by the Dual Boson (DB) formalism [48–51], we construct a bosonic model whose interaction is reminiscent of Anderson’s superexchange mechanism [52,53]. Importantly, the derived formalism remains applicable not only in the strongly localized regime and allows the description of every magnetic system with a well-defined local magnetic moment. Moreover, the presence of the latter allows us to reveal a general way of the description of a complicated quantum many-body problem in terms of single-particle quantities with the use of Ward identities [54,55].

*Effective  $s$ - $d$  model.*—We consider the action of the extended Hubbard model for correlated electrons,

$$S = - \sum_{\mathbf{k}, \nu, \sigma} c_{\mathbf{k}\nu\sigma}^* [i\nu + \mu - \varepsilon_{\mathbf{k}}] c_{\mathbf{k}\nu\sigma} + U \sum_{\mathbf{q}, \omega} n_{\mathbf{q}\omega\uparrow}^* n_{\mathbf{q}\omega\downarrow} + \frac{1}{2} \sum_{\mathbf{q}, \omega, \zeta} \rho_{\mathbf{q}\omega}^* [V_{\mathbf{q}}]_{\zeta\zeta} \rho_{\mathbf{q}\omega}. \quad (1)$$

Here,  $c_{\mathbf{k}\nu\sigma}^*$  ( $c_{\mathbf{k}\nu\sigma}$ ) are Grassmann variables corresponding to creation (annihilation) of an electron with momentum  $\mathbf{k}$ , fermionic Matsubara frequency  $\nu$ , and spin  $\sigma$  labels. The label  $\zeta = \{c, s\}$  depicts charge  $c$  and spin  $s = \{x, y, z\}$  degrees of freedom (d.o.f.), so  $U$  corresponds to local Coulomb interaction,  $[V_{\mathbf{q}}]_{cc} = V_{\mathbf{q}}$  and  $[V_{\mathbf{q}}]_{ss} = -J_{\mathbf{q}}^d/2$  describe nonlocal Coulomb and direct ferromagnetic exchange interactions, respectively. Here, we also introduce bosonic variables:  $\rho_{\mathbf{q}\omega}^{\zeta} = n_{\mathbf{q}\omega}^{\zeta} - \langle n_{\mathbf{q}\omega}^{\zeta} \rangle$ , where  $n_{\mathbf{q}\omega}^{\zeta} = \sum_{\mathbf{k}, \nu, \sigma, \sigma'} c_{\mathbf{k}\nu\sigma}^* \sigma_{\sigma\sigma'}^{\zeta} c_{\mathbf{k}+\mathbf{q}, \nu+\omega, \sigma'}$  is the charge ( $\zeta = c$ ) and spin ( $\zeta = s$ ) density of electrons with the momentum  $\mathbf{q}$ , bosonic frequency  $\omega$ , and Pauli matrices  $\sigma^{\zeta} = \{\mathbb{1}, \sigma^s\}$ .

Expressing the effective exchange interaction in terms of correlation functions is a nontrivial task since it is not an observable. Furthermore, in the strongly correlated regime charge and spin fluctuations are entangled in a complicated way. Both challenges can be approached within the dual boson formalism [48–51] since it naturally separates charge and spin d.o.f. by representing them in terms of bosonic fields entering an effective action. To this aim, one splits the lattice action (1) into the local impurity problem of the extended dynamical mean-field theory (EDMFT [56–61]) and the remaining nonlocal part, which is a bilinear function of  $c^*(c)$  and  $\rho$  variables. Within the DB approach

this remaining part is decoupled by two Hubbard-Stratonovich transformations, thus introducing *dual* fermionic  $f^*(f)$  and bosonic  $\phi$  fields. Then, the initial fermionic d.o.f.  $c^*(c)$  can be integrated out, leading to the interaction part  $\tilde{W}[f, \phi]$  of the resulting dual action being expressed in terms of the full vertex functions of the local impurity problem (for details see the Supplemental Material [62]). Thus, by construction, local correlations are already embedded in the bare propagators and interactions of the DB problem, which is very convenient for practical calculations. In the following we restrict ourselves to the lowest order terms in  $\tilde{W}[f, \phi]$  stemming from the four-point  $\tilde{\gamma}_{\nu\nu'\omega}$  and three-point  $\gamma_{\nu\omega}$  vertices [62].

Dual fields  $f^*(f)$  and  $\phi$  have no direct physical interpretation, but this fact does not represent a significant obstacle for the calculation of physical observables since there is an exact connection between dual and lattice quantities [48–51]. However, for our goal of deriving an effective bosonic model that describes initial (lattice) d.o.f., it is crucial to formulate the problem in terms of bosonic fields that have a clear physical meaning. To remedy this problem, we perform the reverse Hubbard-Stratonovich transformation for the bosonic variables  $\phi$  introducing fields  $\bar{\rho}$ . In this we were inspired by the works of Dupuis [63–65], where a similar trick was performed for fermionic d.o.f. After integrating over dual bosonic fields  $\phi$ , one gets the following action reminiscent of the  $s$ - $d$  model [62]:

$$S_{s-d} = - \sum_{\mathbf{k}, \nu, \sigma} f_{\mathbf{k}\nu\sigma}^* \tilde{G}_0^{-1} f_{\mathbf{k}\nu\sigma} - \frac{1}{2} \sum_{\mathbf{q}, \omega, \zeta'} \bar{\rho}_{\mathbf{q}\omega}^* [X_E]_{\zeta\zeta'}^{-1} \bar{\rho}_{\mathbf{q}\omega}^{\zeta'} + W. \quad (2)$$

Here,  $X_E$  is the EDMFT susceptibility and  $\tilde{G}_0$  is the nonlocal part of the EDMFT Green’s function. Importantly, after all transformations the field  $\bar{\rho}$  indeed has the same physical meaning as the original *composite* bosonic field  $\rho$  of the lattice problem (1), as shown in Ref. [62]. The decisive advantage of the variable  $\bar{\rho}$  is that it can now be treated as the *elementary* bosonic field that has a well-defined propagator and is independent of fermionic d.o.f.  $c^*(c)$ . Remarkably,  $W[f, \bar{\rho}]$  keeps the practical form of the dual interaction  $\tilde{W}[f, \phi]$  with the replacement of bosonic variable  $\phi \rightarrow \bar{\rho}$ , although the four-fermionic term is modified under these transformations. As we argue in Ref. [62] and numerically check below, in the case of well-developed bosonic fluctuations, this modification results in the corresponding contribution to the interaction  $W[f, \rho]$  becoming negligibly small, and the latter takes the simple form  $W[f, \rho] \simeq \sum_{\mathbf{k}, \mathbf{q}} \sum_{\nu, \omega, \zeta} \gamma_{\nu\omega}^{\zeta} \rho_{\mathbf{q}\omega}^* f_{\mathbf{k}\nu\sigma}^* f_{\mathbf{k}+\mathbf{q}, \nu+\omega, \sigma'}$ . At last, we mention that the fermionic d.o.f. are kept in the dual space, which will prove to be useful to discriminate between local and nonlocal contributions to the lattice susceptibility.

**Magnetic susceptibility.**—In order to design an effective Heisenberg model for spin d.o.f., one has to assume that the local magnetization  $\langle m \rangle = 2\langle S^z \rangle$  is described well at the dynamical mean-field level, and fluctuations revealed by the system beyond EDMFT are mostly bosonic. In order to have well-defined local magnetic moment, the effective impurity model has to be considered for the spin-polarized state. For an easier description, one can transform spin variables from the  $\mathbf{s} = \{x, y, z\}$  to the  $\mathbf{s} = \{+, -, z\}$  basis with  $S^\pm = (\rho^x \pm i\rho^y)/2$ . In the spin-polarized case, charge and spin  $z$  channels are yet entangled, but the  $\pm$  spin channel can be separated in the collinear case [66,67]. Thus, for the correct description of the spin fluctuations, one may consider correlations only in the  $\pm$  spin channel, and the contribution of the  $z$  channel to the exchange interaction can later be restored from symmetry arguments. For simplicity,  $\pm$  spin labels are omitted wherever they are not crucial for understanding.

Now, one can integrate out fermionic d.o.f. in the effective action (2) and get the following spin model:

$$\mathcal{S}_{\text{spin}} = -\frac{1}{2} \sum_{\mathbf{q}, \omega} S_{\mathbf{q}\omega}^- [X_{\mathbf{q}\omega}^+]^{-1} S_{-\mathbf{q}, -\omega}^+ + \text{H.c.} \quad (3)$$

A first approximation for the magnetic susceptibility  $X_{\mathbf{q}\omega}$  can be obtained for the case when the interaction  $W[f, \rho]$  contains only the three-point vertex  $\gamma_{\nu\omega}^\pm$ , as discussed above. Therefore, the expansion of the partition function of the action (2) up to the second order with respect to bosonic fields gives [62]

$$[X_{\mathbf{q}\omega}^{(2)}]^{-1} = J_{\mathbf{q}}^d + \Lambda_\omega + \chi_\omega^{-1} - \tilde{\Pi}_{\mathbf{q}\omega}^{(2)}. \quad (4)$$

Here,  $\Lambda_\omega$  and  $\chi_\omega$  are the bosonic hybridization function and susceptibility of the impurity problem, respectively. Also,

$$\tilde{\Pi}_{\mathbf{q}\omega}^{(2)} = \sum_{\mathbf{k}, \nu} \gamma_{\nu+\omega, -\omega}^- \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu+\omega} \tilde{G}_{\mathbf{k}\nu} \gamma_{\nu, \omega}^+ = \text{diagram} \quad (5)$$

is the second-order polarization function [49]. Note that a conserving description of spin fluctuations is given by the two-particle ladder approximation of the magnetic susceptibility provided by the ladder DB approach [50] that accounts for the four-fermion contribution in  $W[f, \bar{\rho}]$  and treats bosonic hybridization  $\Lambda$  as a constant [55]

$$[X_{\mathbf{q}\omega}^{\text{ladd}}]^{-1} = J_{\mathbf{q}}^d + \Lambda + [X_{\mathbf{q}\omega}^{\text{DMFT}}]^{-1}. \quad (6)$$

Here,  $X_{\mathbf{q}\omega}^{\text{DMFT}} = \chi_\omega + \chi_\omega \tilde{\Pi}_{\mathbf{q}\omega}^{\text{ladd}} \chi_\omega$  is the DMFT- [33,34], or dynamical vertex approximation (DGA)-like [68] susceptibility written in terms of local two-particle irreducible four-point vertices and lattice Green's functions.  $\tilde{\Pi}_{\mathbf{q}\omega}^{\text{ladd}}$  is the dual polarization in the ladder form [62,69] that contains  $\tilde{\Pi}_{\mathbf{q}\omega}^{(2)}$  as the lowest order term. Therefore, the hybridization

$\Lambda$  plays the role of the Moriya-like  $\lambda$  correction that was introduced in DGA [70] by hand similarly to the Moriya and Kawabata theory of weak itinerant magnets [71,72] and now is derived analytically.

Importantly, the expressions for magnetic susceptibility (4) and (6) can be drastically simplified to be applicable for realistic multiband calculations, for which the two-particle quantities can hardly be obtained. As was discussed above, the system with a well-defined local magnetic moment exhibits mostly bosonic fluctuations. Therefore, one can expect that local vertex functions are mostly described by the bosonic frequency  $\omega$ , while the dependence on fermionic frequencies  $\nu, \nu'$  is negligible and can be averaged out. In order to perform this averaging consistently, it is carried out using the local Ward identities [54,55], which leads to the following approximation of a three-point vertex [62]:

$$\gamma_{\nu\omega}^+ = \gamma_{\nu+\omega, -\omega}^- \simeq \chi_\omega^{-1} + \delta\Sigma_{\nu\omega} \simeq \chi_\omega^{0-1}. \quad (7)$$

Here,  $\chi_\omega^0 = \sum_\nu g_{\nu+\omega} g_{\nu\omega}$  is the bare spin susceptibility,  $g_{\nu\sigma}$  and  $\Sigma_{\nu\sigma}$  are the full Green's function and self-energy of the impurity problem, and  $\delta\Sigma_{\nu\omega} = (\Sigma_{\nu+\omega\uparrow} - \Sigma_{\nu\downarrow})/\langle m \rangle$ . Therefore, exploiting the system being in the magnetic phase allows us to rewrite the complicated many-body problem (1) in a much simpler form of Eq. (2) introducing bosonic fields that correspond to the collective magnetic fluctuations. In this case, the expression for the corresponding fermion-boson coupling  $\gamma_{\nu\omega}^\pm$  can be drastically simplified (7), leading to a similar expression that was recently postulated in Ref. [73] and numerically checked using brute force calculations [74].

**Exact numerical solution.**—In order to exemplify the above approximations, we consider the half-filled Hubbard model (1) ( $V_{\mathbf{q}}, J_{\mathbf{q}}^d, \Lambda = 0$ ) on the hypercubic lattice in infinite dimensions. In this case, the exact result for the magnetic susceptibility is known to be given by the DMFT

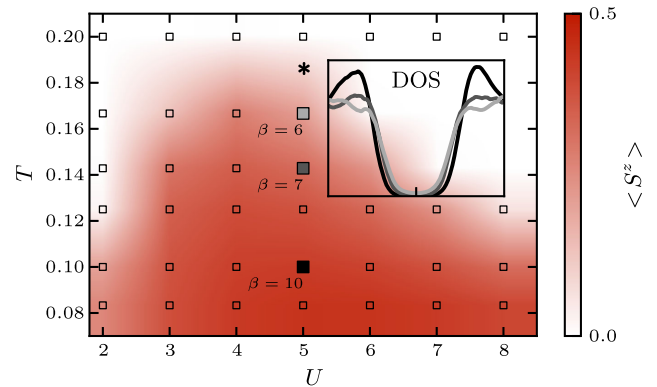


FIG. 1. The antiferromagnetic phase of the half-filled Hubbard model. Squares mark where calculations were done, the red shading depicts the magnitude of the magnetic moment  $\langle S^z \rangle$ , and the asterisk marks the Néel temperature  $T_N \approx 0.186$ . (Inset) The total DOS at  $\beta = 6, 7$ , and  $10$  for  $U = 5$ .

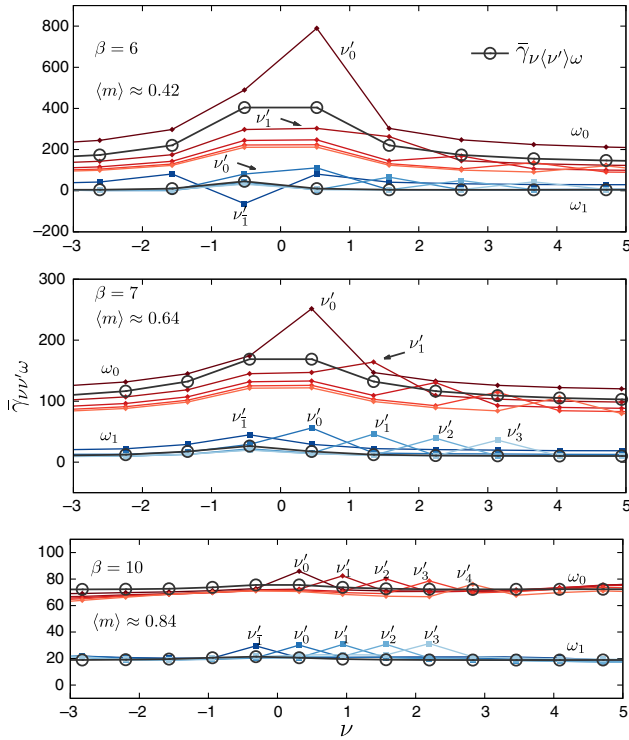


FIG. 2. Real part of the four-point vertex  $\bar{\gamma}_{\nu\nu'\omega}$  in the  $\pm$  spin channel at  $U = 5$  for three different temperatures (see the marked points in Fig. 1). The plot shows  $\bar{\gamma}_{\nu\nu'\omega}$  as a function of  $\nu$  for fixed  $\omega$  and  $\nu'$ . Diamonds and squares show data for  $\omega = \omega_0$  and  $\omega_1$ , respectively. Red ( $\omega_0$ ) and blue ( $\omega_1$ ) lines serve as guides for the eye, whereas lighter colors indicate larger  $\nu'$ . Black circles and lines show  $\bar{\gamma}_{\nu\nu'\omega}$ , which does not depend on  $\nu'$ .

expression (6) and can be compared to the simplified result of Eq. (4). At low temperatures this system favors anti-ferromagnetic (AFM) order over paramagnetism, as shown in the phase diagram in Fig. 1.

The local four-point vertex  $\bar{\gamma}_{\nu\nu'\omega}$  is measured at  $U = 5$  for the three temperatures marked in Fig. 1, roughly below the maximum of the AFM dome, where  $T_N \approx 0.186$  is obtained using the DMFT [62]. As the temperature is lowered from  $\beta = 6$  to  $\beta = 10$ , the magnetization  $\langle m \rangle$  increases from  $\approx 0.42$  to  $0.84$ . We validate in Fig. 2 that at large magnetization the dependence of the four-point vertex  $\bar{\gamma}_{\nu\nu'\omega}$  on fermionic frequencies  $\nu, \nu'$  is small. Consequently, one may indeed use the approximated form of the vertex  $\bar{\gamma}_{\nu\nu'\omega} \simeq \bar{\gamma}_{\nu\nu'\omega}$ , which leads to Eq. (7).

We evaluate Eq. (6) in the AFM phase at the  $\mathbf{q} = 0$  point of the reduced Brillouin zone. The transversal susceptibility is a  $2 \times 2$  matrix with the homogeneous susceptibility  $X^{\text{hom}}(\omega)$  as a diagonal element [75]. Figure 3 shows  $X^{\text{hom}}(\omega)$ , which is real, as well as the off-diagonal element  $X^{\text{off}}(\omega)$ . Remarkably, despite the approximation of the vertex functions,  $X^{\text{hom}}(\omega \neq 0) = 0$  and  $X^{\text{off}}(\omega \neq 0) = -2i\langle m \rangle/\omega$ , which are exact constraints due to global spin conservation [62], hold to very good accuracy.

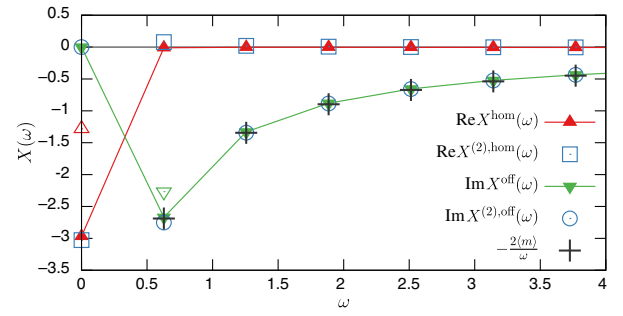


FIG. 3. Spin susceptibility components  $X^{\text{hom}}_\omega$  and  $X^{\text{off}}_\omega$  as a function of the Matsubara frequency (triangles). Squares and circles show the simplified form of the magnetic susceptibility (4). The single red triangles indicate expression for the magnetic susceptibility in the case of the truncated ladder (see the text). The parameters of this figure correspond to the bottom panel of Fig. 2.

At  $U = 5$  the eigenvalue of the ladder equation (6) corresponding to  $X^{\text{hom}}(\omega = 0)$  is large ( $\approx 0.715$ ). Therefore, one can not approximate the polarization  $\tilde{\Pi}^{\text{ladd}}_{\mathbf{q}\omega}$  by the second-order expression  $\tilde{\Pi}^{(2)}_{\mathbf{q}\omega}$  in Eq. (6). The corresponding approximation for  $\text{Re}X^{\text{hom}}(\omega = 0)$  and  $\text{Im}X^{\text{off}}(\omega = 2\pi\beta)$  is marked in Fig. 3 with open triangles and is indeed clearly distinguishable from Eq. (6).

Nonetheless, the simplified expression for magnetic susceptibility  $X^{(2)}$  (4) with the vertex approximation (7) shows a good agreement with  $X^{\text{ladd}}$  (6). Importantly, the approximation for the magnetic susceptibility obtained in Eq. (4) should not be confused with the truncation of the ladder equation, even though it formally uses the same quantity  $\tilde{\Pi}^{(2)}_{\mathbf{q}\omega}$ . The good agreement of the simplified result  $X^{(2)}$  with the much more advanced ladder approximation (6) shows that the bosonic fluctuations indeed dominate in the polarized regime of the impurity model, which was assumed while deriving Eq. (4).

*Classical Heisenberg Hamiltonian.*—Although the action (3) is general and can be used for the description of quantum effects in terms of susceptibilities, at low temperatures it can be mapped onto an effective classical Heisenberg Hamiltonian  $H_{\text{spin}} = -\sum_{\mathbf{q}} J_{\mathbf{q}} \mathbf{S}_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}}$  that describes small spin fluctuations around the AFM ground state [29]. To this aim, spin variables  $S^{\pm}_{\mathbf{q}\omega}$  in Eq. (3) are replaced by classical vectors  $\mathbf{S}_{\mathbf{q}}$  of the length  $\langle S_z \rangle$ , and the contribution from the  $z$  spin channel is restored from the requirement of rotational invariance. Then, an effective exchange interaction  $J_{\mathbf{q}}$  can be defined as a nonlocal part of the inverse spin susceptibility at the zero bosonic frequency [31]. Thus, the effective exchange interaction that corresponds to the simplified form of magnetic susceptibility (4) reads

$$J_{\mathbf{q}} = J_{\mathbf{q}}^d - \sum_{\mathbf{k}, \nu} \gamma_{\nu, \omega=0}^- \tilde{G}_{\mathbf{k}+\mathbf{q}, \nu \uparrow} \tilde{G}_{\mathbf{k}, \nu \downarrow} \gamma_{\nu, \omega=0}^+, \quad (8)$$

while the exchange interaction in the ladder approximation is detailed in Ref. [62]. This result is reminiscent of Anderson's idea of the superexchange interaction



[52,53]. Indeed, the first and the second term in Eq. (8) describe the direct ferromagnetic and kinetic antiferromagnetic exchange interactions, respectively. As a result, in the strongly localized regime and in the case of an antiferromagnetic dimer, the kinetic part of the exchange interaction takes the well-known form  $J = -2t^2/U$  [62].

It is worth mentioning that the three-point vertex  $\gamma_{\nu,\omega}$  that enters the kinetic part of the exchange interaction describes the total spin splitting. In the spin-polarized case, one can again use the simplified form of the vertex function [the first approximation in Eq. (7)]. In the strongly polarized regime, the potential contribution to the spin splitting  $\delta\Sigma_{\nu\omega}$  is much larger than the kinetic one  $\chi_{\omega}^{-1}$ . Therefore, the latter can be neglected and the result for the exchange interaction (8) reduces to the expression obtained in Ref. [31] that was successfully applied to the description of many realistic systems [39–44]. Note that in Ref. [31] the exchange interaction was derived assuming the existence of the collinear spin ground state, while here we show that the limit of applicability of the derived expression is much broader. If the dependence of the three-point vertex on the fermionic frequencies is fully disregarded [the second approximation in Eq. (7)], the exchange interaction reduces to the “Hartree-Fock” approximation  $J_{\mathbf{q}} = \chi_{\omega=0}^{-1} X_{\mathbf{q},\omega=0}^0 \chi_{\omega=0}^{-1}$  [62] derived in Ref. [76].

**Conclusion.**—To conclude, here we derived the action for effective  $s$ – $d$  and Heisenberg-like problems for the extended Hubbard model. We observed that, by virtue of a local Ward identity, the vertex functions of the impurity model can be well approximated, provided its weak dependence on the fermionic frequencies. Our results show that this criterion is indeed satisfied in the AFM phase of the Hubbard model in infinite dimensions when the staggered magnetization is sufficiently large. As a consequence, it is possible to obtain the magnetic susceptibility without a costly measurement of the impurity vertex functions, which is very useful for the realistic multiband calculations. For the considered parameters this approximation becomes accurate enough to reach an agreement with the global spin conservation. In finite dimensions this is of importance for a sound description of magnon spectra in accord with Goldstone’s theorem. In the classical limit, the derived spin action reduces to an effective Heisenberg Hamiltonian. In the spin-polarized case, the result for the kinetic part of the effective exchange interaction simplifies to the expression derived in Ref. [31], which is argued to be a good approximation for the case of many real materials. We believe that this approximation can be applied in different and, in particular, more realistic contexts. We further speculate that similar approximations could prove valuable in any physical regime where it can be argued that the behavior of the vertex functions is strongly dominated by the transferred momentum.

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- [1] A. Bogdanov and D. Yablonskii, *Sov. Phys. JETP* **68**, 101 (1989).
  - [2] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, and P. Böni, *Science* **323**, 915 (2009).
  - [3] X. Yu, Y. Onose, N. Kanazawa, J. Park, J. Han, Y. Matsui, N. Nagaosa, and Y. Tokura, *Nature (London)* **465**, 901 (2010).
  - [4] S. Heinze, K. Von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer, and S. Blügel, *Nat. Phys.* **7**, 713 (2011).
  - [5] F. Jonietz, S. Mühlbauer, C. Pfleiderer, A. Neubauer, W. Münzer, A. Bauer, T. Adams, R. Georgii, P. Böni, R. A. Duine, K. Everschor, M. Garst, and A. Rosch, *Science* **330**, 1648 (2010).
  - [6] A. Fert, V. Cros, and J. Sampaio, *Nat. Nanotechnol.* **8**, 152 (2013).
  - [7] N. Romming, C. Hanneken, M. Menzel, J. E. Bickel, B. Wolter, K. von Bergmann, A. Kubetzka, and R. Wiesendanger, *Science* **341**, 636 (2013).
  - [8] A. Y. Kitaev, *Phys. Usp.* **44**, 131 (2001).
  - [9] A. Kitaev, *Ann. Phys. (New York)* **321**, 2 (2006).
  - [10] C. Beenakker, *Annu. Rev. Condens. Matter Phys.* **4**, 113 (2013).
  - [11] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, *Phys. Rev. Lett.* **105**, 077001 (2010).
  - [12] J. D. Sau, R. M. Lutchyn, S. Tewari, and S. Das Sarma, *Phys. Rev. Lett.* **104**, 040502 (2010).
  - [13] V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, *Science* **336**, 1003 (2012).
  - [14] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, *Science* **346**, 602 (2014).
  - [15] M. Reiher, N. Wiebe, K. M. Svore, D. Wecker, and M. Troyer, *Proc. Natl. Acad. Sci. U.S.A.* **114**, 7555 (2017).
  - [16] W. Heitler and F. London, *Z. Phys.* **44**, 455 (1927).

- [17] A. J. Freeman and R. E. Watson, *Phys. Rev.* **124**, 1439 (1961).
- [18] J. B. Goodenough, *Magnetism and the Chemical Bond*, Vol. 143 (Wiley InterScience, New York, 1964).
- [19] S. V. Vonsovskii, *Magnetism*, Vol. 2 (John Wiley & Sons, New York, 1974).
- [20] V. A. Gubanov, A. I. Lichtenstein, and A. V. Postnikov, *Magnetism and the Electronic Structure of Crystals*, Vol. 98 (Springer Science+Business Media, New York, 2012).
- [21] D. Khomskii, *Transition Metal Compounds* (Cambridge University Press, Cambridge, England, 2014).
- [22] L. Hedin and S. Lundqvist, *Solid State Phys.* **23**, 1 (1970).
- [23] R. O. Jones and O. Gunnarsson, *Rev. Mod. Phys.* **61**, 689 (1989).
- [24] J. Kübler, *Theory of Itinerant Electron Magnetism*, Vol. 106 (Oxford University Press, New York, 2017).
- [25] C. Herring, *Exchange Interactions among Itinerant Electrons: Magnetism*, Vol. 4 (Academic Press, New York, 1966).
- [26] T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer, New York, 1985).
- [27] Y. A. Izyumov, M. I. Katsnelson, and Y. N. Skryabin, *Itinerant Electron Magnetism* (Fizmatlit, Moscow, 1994).
- [28] A. I. Lichtenstein, M. I. Katsnelson, and V. A. Gubanov, *J. Phys. F* **14**, L125 (1984).
- [29] A. Lichtenstein, M. Katsnelson, and V. Gubanov, *Solid State Commun.* **54**, 327 (1985).
- [30] A. Lichtenstein, M. Katsnelson, V. Antropov, and V. Gubanov, *J. Magn. Magn. Mater.* **67**, 65 (1987).
- [31] M. I. Katsnelson and A. I. Lichtenstein, *Phys. Rev. B* **61**, 8906 (2000).
- [32] L. V. Pourovskii, *Phys. Rev. B* **94**, 115117 (2016).
- [33] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).
- [34] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [35] A. Secchi, S. Brener, A. Lichtenstein, and M. Katsnelson, *Ann. Phys. (N.Y.)* **333**, 221 (2013).
- [36] M. I. Katsnelson, Y. O. Kvashnin, V. V. Mazurenko, and A. I. Lichtenstein, *Phys. Rev. B* **82**, 100403 (2010).
- [37] A. Secchi, A. Lichtenstein, and M. Katsnelson, *Ann. Phys. (N.Y.)* **360**, 61 (2015).
- [38] A. Secchi, A. Lichtenstein, and M. Katsnelson, *J. Magn. Magn. Mater.* **400**, 112 (2016).
- [39] K. Sato, L. Bergqvist, J. Kudrnovský, P. H. Dederichs, O. Eriksson, I. Turek, B. Sanyal, G. Bouzerar, H. Katayama-Yoshida, V. A. Dinh, T. Fukushima, H. Kizaki, and R. Zeller, *Rev. Mod. Phys.* **82**, 1633 (2010).
- [40] D. W. Boukhvalov, V. V. Dobrovitski, M. I. Katsnelson, A. I. Lichtenstein, B. N. Harmon, and P. Kögerler, *Phys. Rev. B* **70**, 054417 (2004).
- [41] V. V. Mazurenko, Y. O. Kvashnin, F. Jin, H. A. De Raedt, A. I. Lichtenstein, and M. I. Katsnelson, *Phys. Rev. B* **89**, 214422 (2014).
- [42] Y. O. Kvashnin, O. Grånäs, I. Di Marco, M. I. Katsnelson, A. I. Lichtenstein, and O. Eriksson, *Phys. Rev. B* **91**, 125133 (2015).
- [43] Y. O. Kvashnin, R. Cardias, A. Szilva, I. Di Marco, M. I. Katsnelson, A. I. Lichtenstein, L. Nordström, A. B. Klautau, and O. Eriksson, *Phys. Rev. Lett.* **116**, 217202 (2016).
- [44] I. V. Solovyev, I. V. Kashin, and V. V. Mazurenko, *Phys. Rev. B* **92**, 144407 (2015).
- [45] R. Logemann, A. N. Rudenko, M. I. Katsnelson, and A. Kirilyuk, *J. Phys. Condens. Matter* **29**, 335801 (2017).
- [46] M. I. Katsnelson and A. I. Lichtenstein, *J. Phys. Condens. Matter* **16**, 7439 (2004).
- [47] A. Secchi, A. I. Lichtenstein, and M. I. Katsnelson, *Phys. Rev. B* **94**, 085153 (2016).
- [48] A. Rubtsov, M. Katsnelson, and A. Lichtenstein, *Ann. Phys. (N.Y.)* **327**, 1320 (2012).
- [49] E. G. C. P. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, and H. Hafermann, *Phys. Rev. B* **90**, 235135 (2014).
- [50] E. A. Stepanov, E. G. C. P. van Loon, A. A. Katanin, A. I. Lichtenstein, M. I. Katsnelson, and A. N. Rubtsov, *Phys. Rev. B* **93**, 045107 (2016).
- [51] E. A. Stepanov, A. Huber, E. G. C. P. van Loon, A. I. Lichtenstein, and M. I. Katsnelson, *Phys. Rev. B* **94**, 205110 (2016).
- [52] P. W. Anderson, *Phys. Rev.* **115**, 2 (1959).
- [53] T. Yildirim, A. B. Harris, A. Aharony, and O. Entin-Wohlman, *Phys. Rev. B* **52**, 10239 (1995).
- [54] H. Hafermann, E. G. C. P. van Loon, M. I. Katsnelson, A. I. Lichtenstein, and O. Parcollet, *Phys. Rev. B* **90**, 235105 (2014).
- [55] F. Krien, E. G. C. P. van Loon, H. Hafermann, J. Otsuki, M. I. Katsnelson, and A. I. Lichtenstein, *Phys. Rev. B* **96**, 075155 (2017).
- [56] A. M. Sengupta and A. Georges, *Phys. Rev. B* **52**, 10295 (1995).
- [57] Q. Si and J. L. Smith, *Phys. Rev. Lett.* **77**, 3391 (1996).
- [58] J. L. Smith and Q. Si, *Phys. Rev. B* **61**, 5184 (2000).
- [59] R. Chitra and G. Kotliar, *Phys. Rev. Lett.* **84**, 3678 (2000).
- [60] R. Chitra and G. Kotliar, *Phys. Rev. B* **63**, 115110 (2001).
- [61] S. Biermann, F. Aryasetiawan, and A. Georges, *Phys. Rev. Lett.* **90**, 086402 (2003).
- [62] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.121.037204> for explicit derivation of the bosonic action and Heisenberg Hamiltonian for spin degrees of freedom of the extended Hubbard model.
- [63] N. Dupuis and S. Pairault, *Int. J. Mod. Phys. B* **14**, 2529 (2000).
- [64] N. Dupuis, *Nucl. Phys.* **B618**, 617 (2001).
- [65] N. Dupuis, [arXiv:cond-mat/0105063](https://arxiv.org/abs/cond-mat/0105063).
- [66] N. Bickers and D. Scalapino, *Ann. Phys. (N.Y.)* **193**, 206 (1989).
- [67] M. I. Katsnelson and A. I. Lichtenstein, *J. Phys. Condens. Matter* **11**, 1037 (1999).
- [68] A. Toschi, A. A. Katanin, and K. Held, *Phys. Rev. B* **75**, 045118 (2007).
- [69] H. Hafermann, E. G. C. P. van Loon, M. I. Katsnelson, A. I. Lichtenstein, and O. Parcollet, *Phys. Rev. B* **90**, 235105 (2014).
- [70] A. A. Katanin, A. Toschi, and K. Held, *Phys. Rev. B* **80**, 075104 (2009).
- [71] T. Moriya and A. Kawabata, *J. Phys. Soc. Jpn.* **34**, 639 (1973).
- [72] T. Moriya and A. Kawabata, *J. Phys. Soc. Jpn.* **35**, 669 (1973).

- [73] M. S. Scheurer, S. Chatterjee, W. Wu, M. Ferrero, A. Georges, and S. Sachdev, Proc. Natl. Acad. Sci. U.S.A. (to be published).
- [74] W. Wu, M. S. Scheurer, S. Chatterjee, S. Sachdev, A. Georges, and M. Ferrero, *Phys. Rev. X* **8**, 021048 (2018).
- [75] The second diagonal element corresponds to  $\mathbf{q} = (\pi, \dots, \pi)$  of the regular Brillouin zone and is divergent due to the rotational invariance of the Hamiltonian.
- [76] V. Antropov, *J. Magn. Magn. Mater.* **262**, L192 (2003).
- [77] I. Krivenko, <https://github.com/krivenko/som>.
- [78] A. S. Mishchenko, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, *Phys. Rev. B* **62**, 6317 (2000).
- [79] E. Gull, S. Isakov, I. Krivenko, A. A. Rusakov, and D. Zgid, [arXiv:1805.03521](https://arxiv.org/abs/1805.03521).
- [80] J. Otsuki, *Phys. Rev. B* **87**, 125102 (2013).